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MFIX Validation Studies December 1994 to November 1995

CRADA No. PC94-026

January 1998

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Executive Summary

Presented are validation results for MFIX, a finite difference, transient code that solves the equations of transport for interacting fluid and granular phases. The predictions of MFIX are compared to four different experimental studies involving the behavior of fluid beds. MFIX correctly predicts much of what is observed, for example, bubble formation, jet penetration lengths, solids circulation cells, mixing of gases and solids, transitions to different flow regimes, pressure and temperature fluctuations, and chemistry involving coal. Occasionally the details are imperfect; for example, the leading edges of bubbles often exhibit spikes, bubble frequency is higher than found experimentally, and flow regime transitions are displaced from the experimentally determined conditions.

Introduction

MFIX is a finite difference, three-dimensional FORTRAN code that solves the equations of transport for mass, momentum, and energy for interacting granular and fluid phases. MFIX has been adapted to fluidized beds by the Morgantown Energy Technology Center (METC) from KFIX, a code used to model the interactions of water and steam in a nuclear reactor.

MFIX is continuously evolving to become more robust and physically correct. Currently its stress tensor incorporates relationships derived using the kinetic theory of gases such as granular temperature. Its drag law spans low to high particle Reynolds number flow. It can perform one-, two-, or three-dimensional simulations and can handle multiple solid phases. It has chemistry for the major constituents involved in coal combustion and gasification and a Prandtl mixing length model for gas phase turbulence. Anticipated refinements to MFIX include a description of incipient and dense granular flows and descriptions of the chemical kinetics of fluid catalytic crackers and biomass gasifiers.

Each modification to MFIX occasions validation studies. The goal is to identify the strengths and weaknesses of MFIX so that it can become an acceptable and reliable design and scale-up tool used by industry. These studies have shown that MFIX captures many features of fluid beds. MFIX predicts bubbles and their growth and coalescence, mixing of solids and fluid, circulation cells, fluctuating pressure drop, fluctuating temperature, flow regime transitions, product gas composition, exit gas heating value, and most other observed aspects of fluid beds.

This report concerns validation studies performed by Foster Wheeler Development Corporation (FWDC) and METC. Four experimental investigations involving fluid beds were used. They featured a variety of geometries and operating conditions: Yang and Keairns (1980); Schmidt, et al. (1988); He, et al. (1995); and Foster Wheeler Development Corporation 10" Carbonizer Experimental Run #TR8.9, Z. Fan (Oct. 1995b).

Validation Studies

Yang and Keairns (1980):

The experimental apparatus used by Yang and Keairns (1980) was a half cylindrical bed about 14 cm in radius. The bottom 15 cm of their apparatus was an inverted, half frustrum. Both air and granular material were introduced vertically through a nozzle, whose center was located about 2 cm inward from the flat side of the half cylinder at the bottom of the inverted frustrum. Additional fluidizing air was introduced through the sloped side of the frustrum. The apparatus was not cylindrically symmetrical about the nozzle center, but did have a vertical plane of symmetry passing through the nozzle. Several experimental runs were made. MFIX was used to simulate six of them, spanning the operating conditions:

Run	Jet Flow m^3/min	Fluidizing Air m^3/min	Jet Velocity m/s	Solids Loading in the Jet wt s./wt g.
GSF-1	1.80	1.78	62.5	0
GSF-5	1.80	1.78	62.5	1.52
GSF-44	0.99	1.78	34.5	0
GSF-45	0.99	1.78	34.5	0.71
GSF-46	0.99	1.78	34.5	1.67
GSF-47	0.99	1.78	34.5	2.75

The simulations were done in a variety of ways to investigate different aspects of the model: two- and three-dimensional geometries, coarse and fine tessellation, and differing gas turbulence strengths were examined.

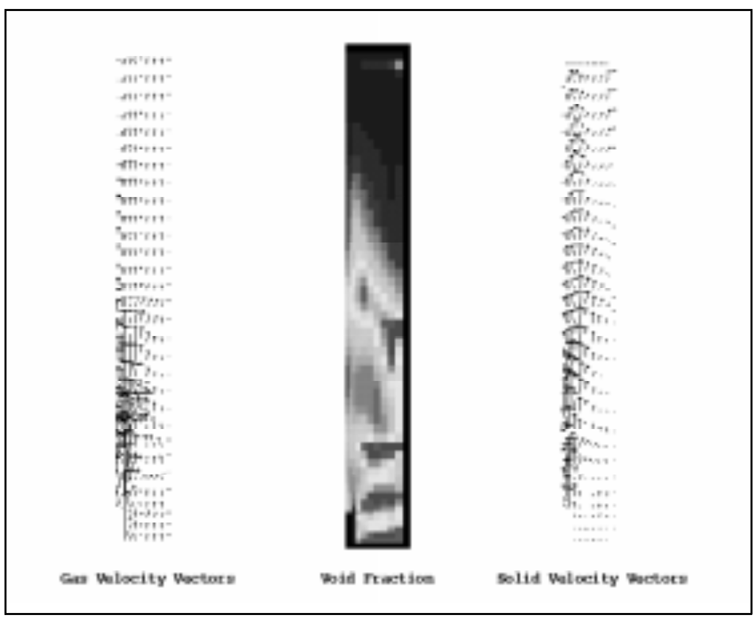

Figure 1: Run GSF-1 at 8.0 seconds

Figure 1, Yang and Keairns (1980) Run GSF-1, shows a snapshot taken at 8.0 s of a typical result for a three-dimensional simulation of experiment GSF-1. The flat wall across the diameter of the cylinder is to the left in each panel, and the curved wall is to the right. Each panel shows the same vertical slice through the symmetry plane of the fluid bed. The void fraction is shown in the center panel - the darker the region, the larger the void fraction. The nozzle is the short vertical gray line offset from the lower left corner. This snapshot suggests the formation of a bubble just above the nozzle. A little later the jet will pinch off, and the bubble will separate. The left panel shows the instantaneous gas velocity vectors. Gas generally moves straight up with some deviation above the jet and around the bubble. Gas preferentially flows through regions of lower particle concentration. The right panel shows the solid velocity vectors. They show two circulation cells, one just above the nozzle and a larger one in the central section of the bed. Both cells rise above the nozzle and sink at the outside wall. Because MFIX calculates all the field variables at every location at every instant, other slices through the bed and other variables can be displayed if desired.

To save time, a two-dimensional simulation of a Yang and Keairns experiment can be performed rather than a three-dimensional simulation. Information found from the two-dimensional simulation can offer insight into the performance of the apparatus and can be usefully compared to experimental results. A two-dimensional simulation of the Yang and Keairns apparatus implies that the nozzle opening is stretched from a small half circle into an annulus extending the entire azimuthal range, 0 through π. This then requires a choice between matching the area of the nozzle opening to the actual nozzle opening or matching its radial extent to its actual value. A further choice exists between either fitting the model inlet velocity to the experimental velocity or fitting the momentums. What makes most sense and seems to duplicate best the experimental data is to keep the nozzle area and inlet volumetric flow the same as the experimental condition. Doing so, however, makes the radial extent of the jet inlet much thinner. If the region around the inlet is of particular interest, only a three-dimensional simulation would be satisfactory.

Interpolating between grid points is a practical problem in comparing numerical results to experimental data. Initially cubic spline interpolation of the gas velocity was used because it matches both data and slope at each grid point. Practice, though, soon proved that the rapid variation in gas velocity near the jet introduced spurious negative gas velocities in the outer jet envelope, so linear interpolation of the data was used instead.

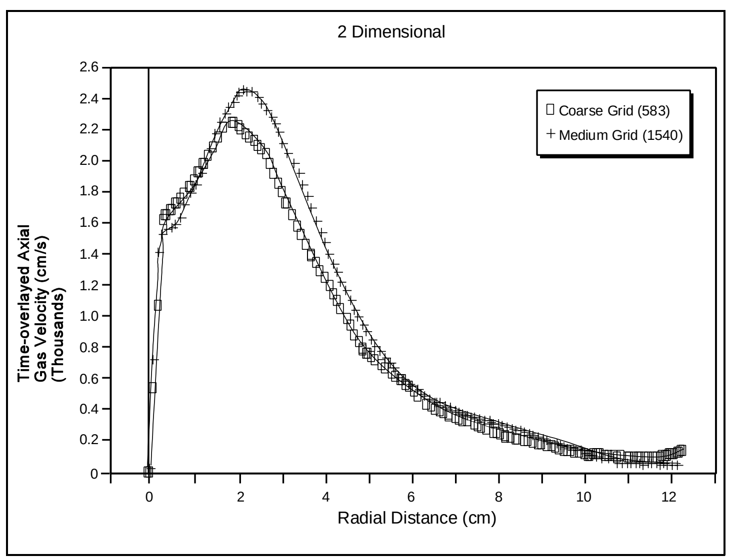

Figure 2: Effect of Tesselation

Figure 2 shows the effect of grid size on the axial, time-averaged, gas velocity profile at 44.5 cm above the nozzle as found from a two-dimensional simulation. It compares results for the average, axial, gas velocity as found from a medium grid consisting of 563 cells and a coarse grid consisting of 154 cells. Conditions were similar to experimental run GSF-1. The velocity of the injected gas and the radial extent of the nozzle were the same as the experimental conditions, but the momentum and volumetric gas flow were not. Figure 2 shows that the medium grid predicts the average axial gas velocity to be more narrowly distributed across the radial direction than does the coarse grid.

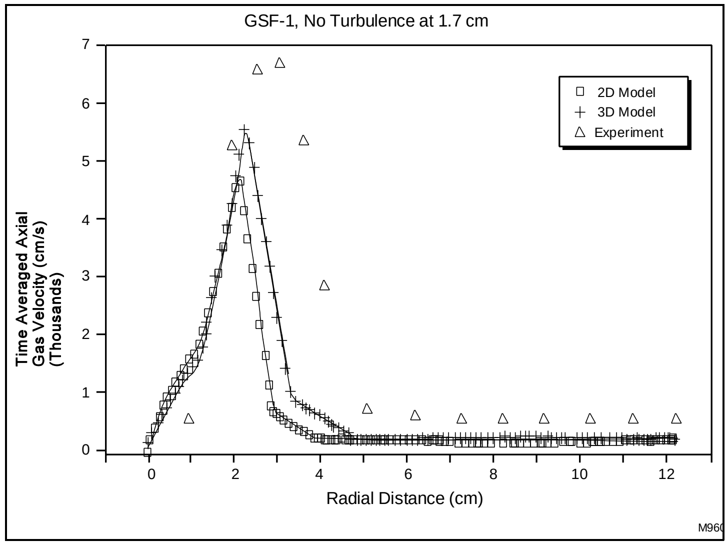

Figure 3: Effect of Dimension (2D vs. 3D)

The results for the time-averaged, axial, gas velocity in the absence of gas phase turbulence as simulated for two-dimensional and three-dimensional cases are compared to the GSF-1 experimental results in figures 3 and 4. As figure 3 indicates, just above the nozzle the two dimensional results are similar to the three-dimensional results, and both show a shoulder near the flat wall which is not reported by experiment. Higher up in figure 4, the shoulder becomes a peak for the three-dimensional simulation, whereas the two-dimensional simulation still retains a shoulder near the flat wall and a peak velocity over the nozzle. Figures 3 and 4 suggest that the total gas flow predicted by MFIX is far less than that shown by experiment. MFIX conserves mass and hence volume, save for the slight increase caused by gas expansion. Probably the experimentally reported gas velocities for GSF-1 are too great since they are inconsistent with the stated inlet conditions. Ignoring for the moment the effect of void fraction on the volumetric flow rate and integrating under the velocity profiles, the model predicts a total flow of 4.9 m^3/min, whereas the experiment predicts a much larger total flow of 12 m^3/min. These numbers compare to a nominal total flow for Run GSF-1 of 3.58 m^3/min. The discrepancies between the model predictions and the nominal flow can be explained by assuming an average void fraction of around 0.7, a reasonable number. The void fraction for the experiment would have to be an unphysical 0.23 to account for such large gas velocities. Yang and Keairns (1980) do not report gas velocity away from the centerline of the apparatus. Perhaps gas preferentially moves towards the centerline, which causes a large axial gas velocity there and a concomitant smaller velocity far from the centerline. The phenomenon would have to be large, though, because 12 m^3/min is over 3 times 3.58 m^3/min.

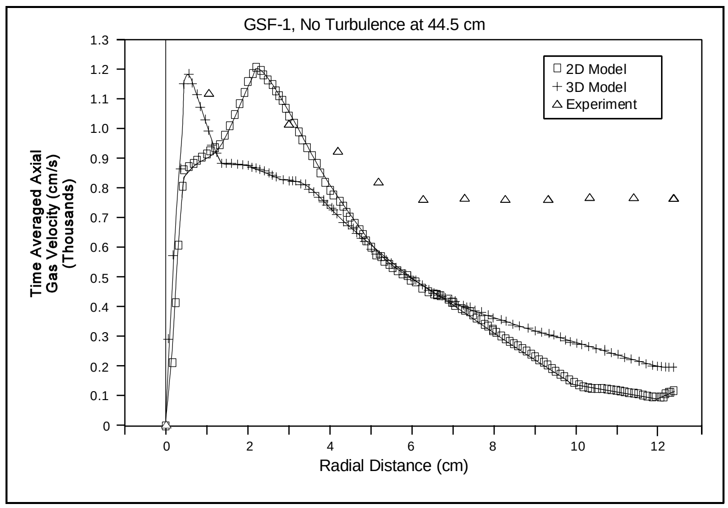

Figure 4: Effect of Dimension (2D vs. 3D)

Yang and Keairns (1980) infer gas velocity from pitot tube measurements. Such inferences require that streamlines exist and that flow energy be constant along them. Simulations show, however, that gas streamlines follow solid streamlines only rarely and then only in a time-averaged sense. Large velocity gradients in the radial direction exist above the nozzle, and energy is dissipated by both gas phase turbulence and particle-particle collisions. Further MFIX simulations were performed mimicking the pitot tube experiment. No consistent relationship was found between the gas velocity given directly by MFIX and the gas velocity inferred from values of the simulated pitot tube measurements. Yang and Keairns (1980) note that the solids momentum in the emulsion phase could affect the pitot tube measurements; they summarize, "Thus the gas velocity reported in the emulsion phase is probably high, but the velocities in the jet region are believed to be accurate."

Figure 4 indicates that the model results are more accurate than the experimental results for the axial, centerline gas velocity for the region distant from the nozzle. Figure 4 also indicates that the axial, centerline, gas velocity in the region above the nozzle as calculated from the three-dimensional simulation is narrower than that found by experiment. This is expected because gas phase turbulence was not included in this simulation. If it had been considered, then the model would have predicted a broadening of the gas velocity profile.

The gas phase turbulence model used in MFIX is based on Prandtl's mixing length theory. It employs a maximum turbulent viscosity parameter, m, taken to be 0.02 poise and a mixing length parameter, l. Experiments done by Tsuji, et al. (1988) of a particle laden jet expanding downward into still air were simulated to validate the simple turbulence model in MFIX. A series of runs was performed using polystyrene beads with mean diameter from 170 to 1400 μ, and a particle-to-air-mass flow ratio ranging from 0.39 to 1.85. The particle velocity was measured directly using laser Doppler velocimetry (LDV), and the gas velocity was taken to be the velocity of entrained, fine ammonium chloride, also measured by LDV.

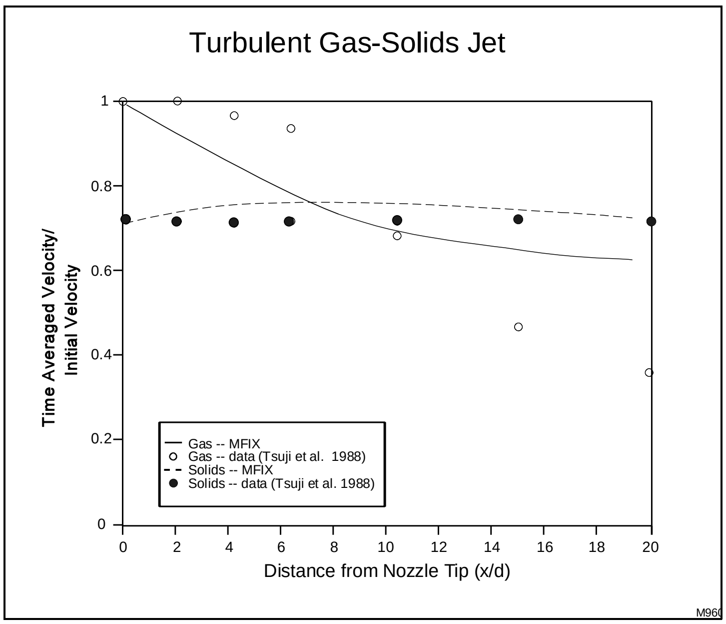

Figure 5: Tsuji, et al. (1988)

Figure 5, Turbulent Gas-Solid Jet, compares the measured axial solids and gas velocities to the MFIX predictions. The predicted solids velocity does well, but that for the gas decelerates too quickly near the nozzle tip and not quickly enough at greater distances from the nozzle tip. A mixing length of 0.8 cm is used in the comparison, but the general shapes of the MFIX profiles do not change significantly with other values of l.

Returning to the Yang and Keairns (1980) jetting bed experiments, one would expect that the larger the mixing length the greater the turbulence and the sooner the jet would be dissipated. Although small, this effect is found by MFIX in both two-dimensional and three-dimensional simulations. Figures 6 and 7 show that the predicted gas velocities in the jet region are similar to those of experiment. As with the no-turbulence simulations presented in figures 4 and 5, MFIX correctly predicts a much smaller gas velocity outside the jet than found experimentally.

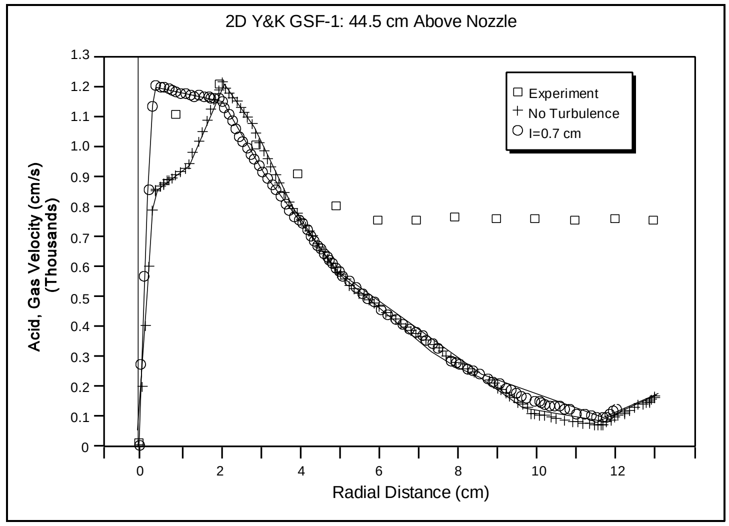

Figure 6: Effect of Turbulence

The effect of the turbulence model is not large because the major mechanism for the dissipation of the jet is momentum exchange from the gas to the solid phase, which occurs even without turbulence. Figure 7 indicates that the mixing length value affects the gas velocity profile only a little just above the nozzle. The effect of the mixing length value increases the longer the gas is in the flow. In figure 8 at 44.5 cm above the nozzle, the effect is discernable with l=0.14. In figure 7, the effect is noticeable only for l=0.80.

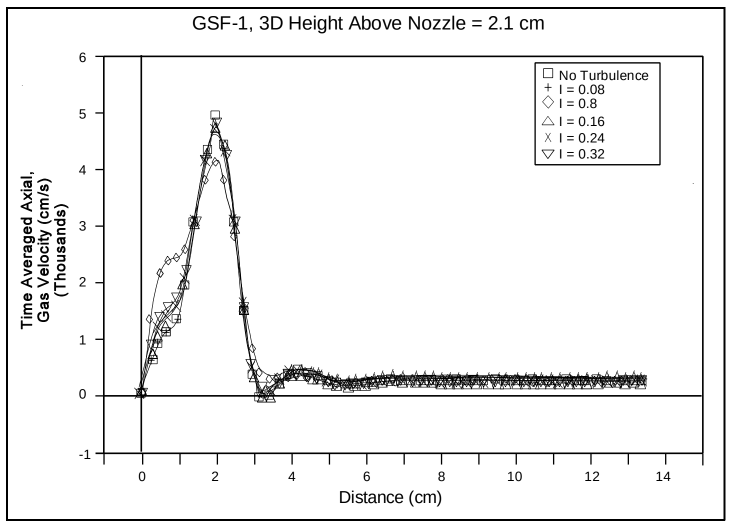

Figure 7: Effect of Turbulence Mixing Length

Yang and Keairns (1980) discovered that their experimentally determined jet profiles closely track Tollmein's universal jet profile (Abramovich, 1963) for a jet expanding into still air. The solid lines in figures 9 and 10 are the Tollmein representations. They are taken to be that for the experimental results as well. The symbols are the MFIX results. The distance r' is the radial distance from the center of the jet normalized by the radial distance at half maximum velocity $r_{1/2}$. U(r') is the gas velocity at r'. U_m is the maximum gas velocity at that axial location, and U_b is the gas velocity above the grid and far from the nozzle. The model predictions for the no-turbulence, two-dimensional simulations consistently show a jet that spreads out less rapidly than that suggested by Tollmein.

Including gas phase turbulence causes the gas velocity profiles to be blunter and match more closely the Tollmein predictions. Figure 11 compares the Tollmein gas velocity profile to the MFIX generated profile for different values of l at 44.5 cm above the nozzle. As turbulence increases, the gas velocity profile becomes blunter. The results imply that MFIX ought to use a mixing length value l≈0.10 to most closely match Tollmein's universal gas velocity profile. However, the resulting predicted profile would still not exactly match Tollmein's for the entire radial domain. The model gas velocity profile would be faster than Tollmein's over the jet and slower away from it.

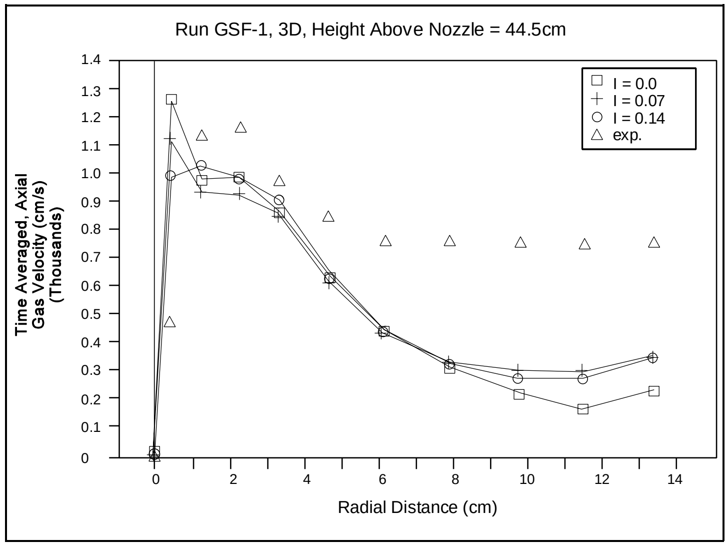

Figure 8: Effect of Turbulence Mixing Length

This difference between model prediction and experimental behavior is similar to that presented earlier in figure 5 comparing two-dimensional MFIX predictions to Tsuji, et al. (1988) experiments. Together, figures 5 and 11 show that a Prandlt mixing length type turbulence model is adequate for many simulations unless a great deal of accuracy is needed. Furthermore, the three-dimensional results in figure 11 are quite similar to the no-turbulence two-dimensional results presented in figures 9 and 10. Thus, the faster two-dimensional, no-turbulence simulations might be adequate for many purposes.

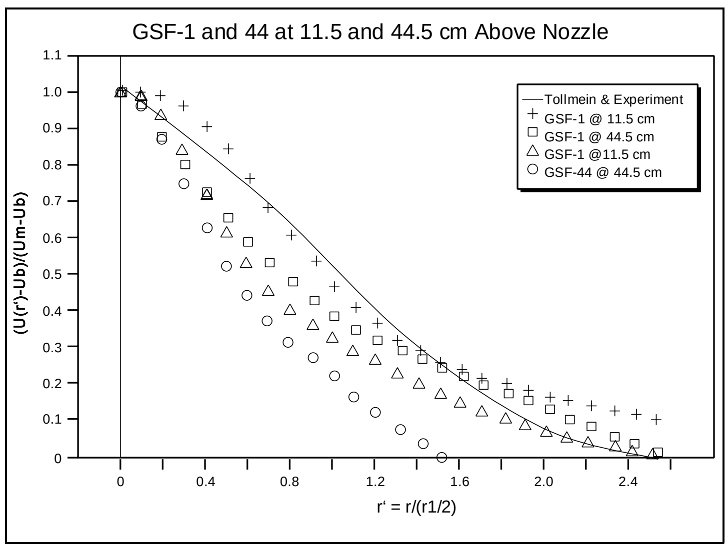

Figure 9: Jet Profiles

Yang and Keairns (1980) quantify the rate at which the jet dissipates by correlating $r_{1/2}$ with the height above the nozzle. Their correlation is given by their equation 2

$$r_{1/2} = 0.0467\ x + \frac{D_T}{2} ,$$

where D_T is the effective nozzle diameter (cm) and x is the height above the nozzle (cm). The dashed line in figure 12, Jet Spreading Rate, is their correlation. Also shown are the two-dimensional, no-turbulence, MFIX results for several experimental conditions as well as the best fit line for each condition. We were curious about the fact that the experimentally determined correlation did not depend upon the initial momentum of the jet. It seemed to us that a jet would dissipate more slowly if it had a larger initial momentum. We noted that the jet spreading rate for run GSF-44 is much faster than the others presented in figure 12, and that its initial jet momentum is less than all the others. Figure 13 summarizes our finding. We learned that the MFIX prediction for $r_{1/2}$ based on two-dimensional simulations without gas phase turbulence could be best correlated by the equation

$$r_{1/2} = \frac{D}{2} + \frac{0.0407}{(p_{gas} + 0.5\ p_{soli}}$$

where p_i is the initial momentum of phase i in the jet.

Figure 14, Eqn. 3 for GSF-47, and figure 15, Eqn. 4 and Computer Model: A/A_o, are shown for completeness. They are correlations determined by Yang and Keairns (1980) from their data. Their equation 3 describes the ratio of the average jet velocity to the maximum jet velocity at a given height above the nozzle:

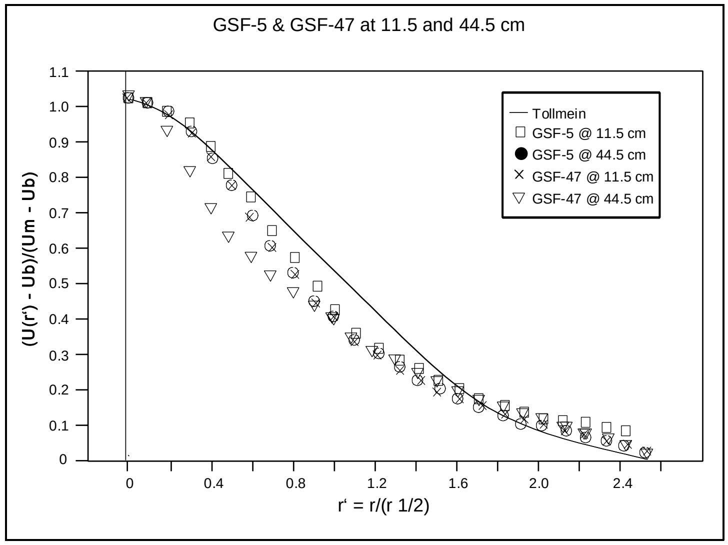

Figure 10: Comparison of Jet Profiles to Tollmein

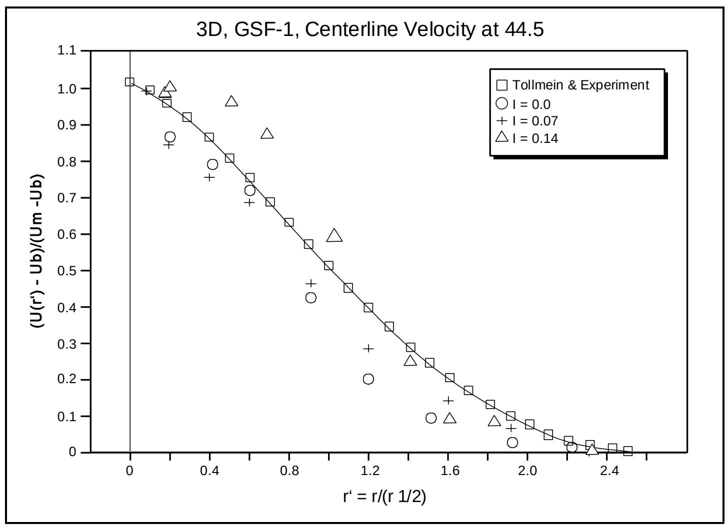

Figure 11: Effect of Turbulence on Jet Profile

$$\frac{U_j}{U_m} = 0.311 + (0.190 - 0.0323R)\ \frac{x}{D_T}\ . \quad 9.3\ \text{cm} \leq x \leq 33.8\ \text{cm}\ ,$$

where U_j is the average jet velocity at height x, U_m is the maximum jet velocity at that height, and R is the solids loading. Since an average can never be more than the maximum, this ratio should never be more than 1. As figure 14 shows, however, equation 3 predicts a value greater than 1. Similarly, the Yang and Keairns (1980) correlation for the ratio of areas under a jet, their equation 4, can never be negative, and yet the correlation is less than zero within the domain of use, as shown in figure 15 and given by their equation 4,

$$\frac{A}{A_0} = 1.486 - 0.0247 \frac{x}{D_T} + 0.165 \ R \ ,$$

where A is the area of the jet at height x and A_0 is nozzle area. In contrast, the model predictions show a ratio that is always greater than zero.

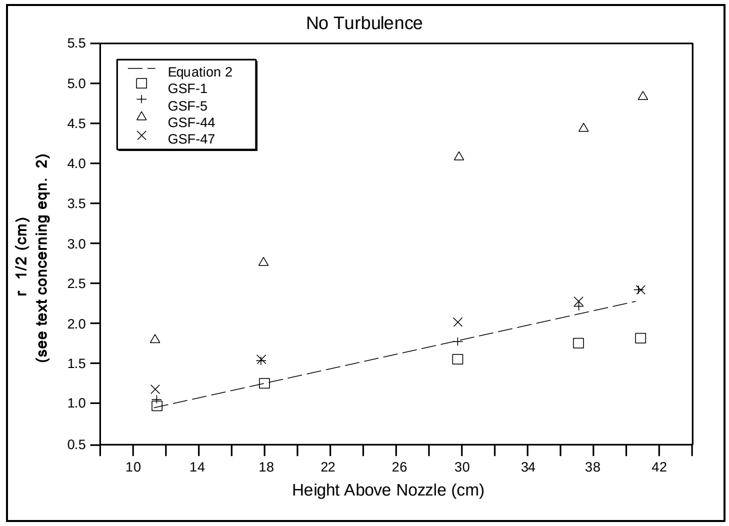

Figure 12: Jet Spreading Rate

Schmidt, et al. (1988):

Westinghouse, Inc., carried out a series of experimental runs on jetting fluid beds (Schmidt, et al., 1988). A half cylindrical vessel, 3 m in diameter and 9.14 m tall, was used. Gas was injected through a 10" nozzle for some runs, and through a 16" nozzle for other runs. Bed depths varied from 4 to 6.1 m, gas velocities to 1.4 m/s, and particle sizes to 0.64 cm. Two-dimensional simulations of Runs TP-M005-3 #12, TP-M005-3 #24, and TP-M011 #7 have been simulated. The operating conditions were:

Run	TP-M005-3	TP-M005-3	TP-M011
Set Point	#12	#24	#7
Air Tube (m^3/min)	16.0	16.3	66.5
Annulus (m^3/min)	10.3	9.7	10.5
Shroud (m^3/min)	4.5	4.3	4.6
Grid-1 (m^3/min)	14.4	14.4	14.3
Grid-3 (m^3/min)	28.6	28.3	28.4
Grid-5 (m^3/min)	52.8	52.1	51.2
Trans Air (m^3/min)	10.5	10.7	9.2
Solid Flow (kg/hr)	0	4631	2776
Freeboard V_g (m/s)	0.63	0.65	0.79
Bed Height (m)	4.0	4.0	5.5
CO_2 Trace Gas (m^3/min)			6.1

Figure 16 shows a snapshot taken at 6.5 s of a two-dimensional simulation of Westinghouse's experiment TP-M005-3 #12. As with figure 1, the left panel is the gas velocity, the center panel is the voidage, and the right panel is the solids velocity. The center panel shows the jet about to pinch off and form a bubble. MFIX's bubble size is about right, but its shape is shown to have a pointed leading edge. Subsequent investigations of the bubble shape in other, simpler geometries suggest that the sharpness of the bubble is <u>not</u> caused by the centerline boundary condition, the grid spacing, the dimension of the simulation, or insufficient solids viscosity. The discrete particle simulations performed by Gera and Tsuji (1997) predict rounded bubbles. The discrete particle method includes the moment of inertia of the individual particles, and it treats the collision between two particles in much greater detail than does MFIX. It also uses a different solution technique. Subsequent modifications to MFIX have shown that the pointed leading edge of bubbles is caused by first order upwinding. Implementation of a higher order discretization scheme in MFIX has fixed the problem, so MFIX now predicts rounded leading edges on bubbles (Syamlal 1997).

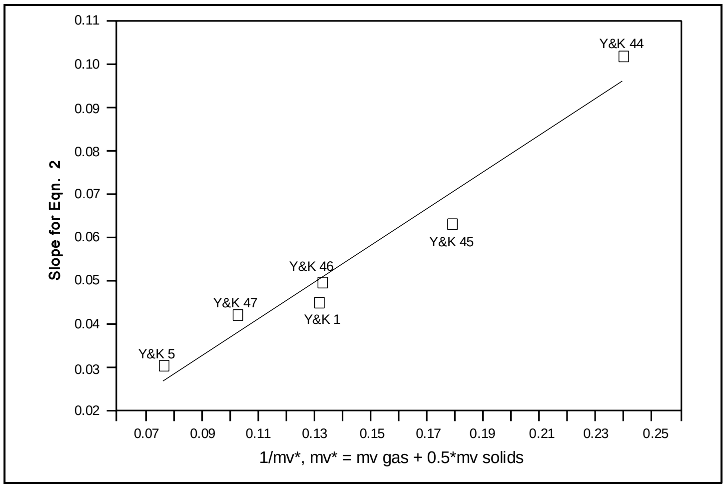

Figure 13: Best Fit on Eqn. 2 Slope
B = 0.0, m = 0.407

Fan (Oct. 1995a) prepared a Table comparing results between the Westinghouse experiments and the corresponding MFIX two-dimensional simulations. In the following Table, the MFIX values are reported on one line and the experimental values are immediately underneath:

Run	TP-M005-3	TP-M005-3	TP-M011
Set Point	#12	#24	#7
Bubble Frequency (1/min) MFIX	117	125	103
Exp.	57	65	
Bubble Diameter (m) MFIX	0.8	0.6	0.7
Exp.	0.79	0.9	
Jet Penetration (m) MFIX	1.98	1.25	2.6
Exp.	1.26	1.25	

The MFIX predicted jet penetration is 1.98 m, whereas the experimental value is 1.26 m. The simulated bubble frequency is 117 bubbles/min, which is about twice the experimental value of 57 bubbles/min. The discrepancy between the model and experimental bubble frequencies indicates that MFIX predicts the leakage of gas from the bubble to be less than found experimentally.

He, et al. (1995):

He, et al. (1995) investigated the behavior of spouting fluid beds in both half cylindrical and full cylindrical geometries. The diameters of the two vessels are 15.2 cm, and their bed heights are both 1.4 m. Each configuration has one source of fluidizing air — a single inlet orifice, 1.9 cm in diameter, positioned along the cylindrical axis at the vertex of its base. The bed in each vessel is composed of closely sized glass beads 1.41 mm in diameter and is 32.5 cm deep. Superficial gas velocities are 59.4, 64.8, and 70.2 cm/s. The extent of the spout, the shape of the bed, and the velocity of the particles are reported. Figure 17, He, et al. (1995), shows an instant during a two-dimensional simulation of the full cylinder experiment.

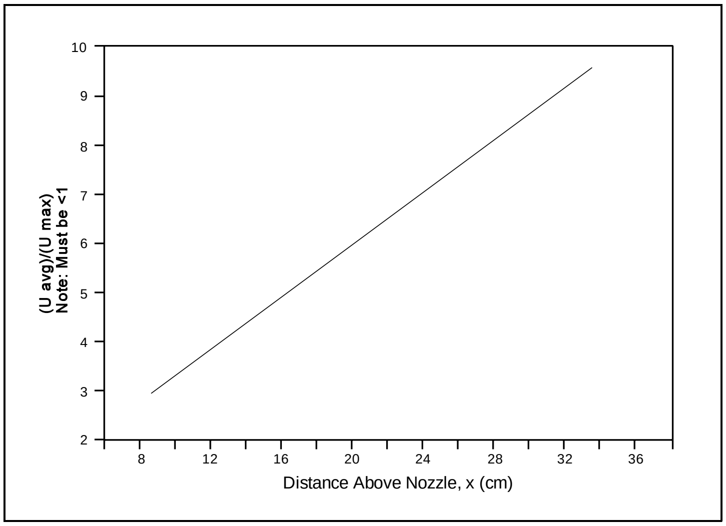

Figure 14: Eqn. 3 for GSF-47

MFIX does not predict the experimentally seen spouting bed behavior. Instead, it predicts a jetting/bubbling bed. Several variations in the operating conditions and modifications of MFIX were tried in order to generate spouting behavior, all without success. Fine, medium and coarse grids were tried. Gas velocities different from the nominal velocity of 38 m/s were tried: 44.91 m/s, 48 m/s, 55 m/s, 65 m/s, and 76 m/s. At the lower gas velocities, the bed exhibited a jet that would disappear a few centimeters into the bed; at the higher gas velocities, the jet would break off and form bubbles. None of the simulated gas velocities evinced spouting bed behavior. The particle size was decreased by 20% from the nominal value to no effect. One simulation started with a spouting bed to determine if multiple solutions were possible and MFIX was converging on an alternative solution. The resulting steady state was the same jetting behavior as found from the nominal starting conditions, implying no alternative solution. The frictional flow regime stress tensor, which mimics dense, granular flow, was extended to higher voidages, but spouting behavior was not observed. Viscosity of the solid phase under the frictional flow regime was increased 10,000 fold, but the steady state behavior remained jetting/bubbling. For some runs, gas phase turbulence was turned on and the mixing length value was varied, but the resulting steady state behavior again was jetting/bubbling. The solids stress tensor

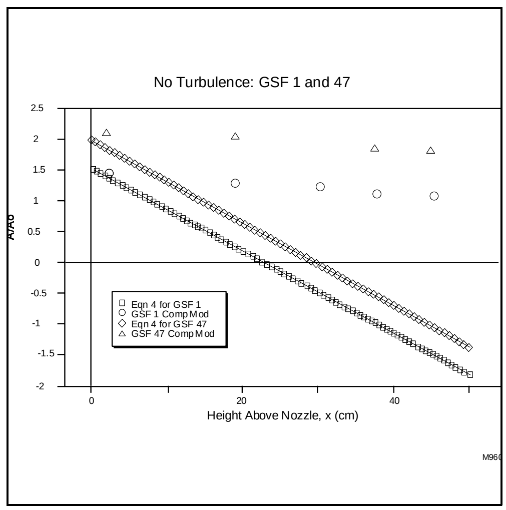

Figure 15: Eqn. 4 and Computer Model: A/Ao

expression in MFIX was modified to include a dependence on the gradient of void fraction, but the resulting behavior was not spouting. A three-dimensional simulation was tried, but the results were that of the two-dimensional simulations, jetting/bubbling behavior. Fan (Oct. 1995b) tried running MFIX with a bed height half the experimental value, but still spouting behavior was not observed.

Several different simulations were executed with the commercial code FLUENT. Excepting a more complicated gas phase turbulence model and body-fitted coordinates, FLUENT shares the same physical assumptions as MFIX but has a different solution algorithm. Gas phase turbulence was turned off, but tessellation was varied, particle size was varied, and both two-dimensional and three-dimensional simulations were done. As with MFIX, FLUENT always predicted a jetting/bubbling bed instead of a spouting bed. Thus, neither the solution algorithm employed by MFIX nor its stairstep representation of the conical bottom is the source of the difference with the He, et al. (1995) study.

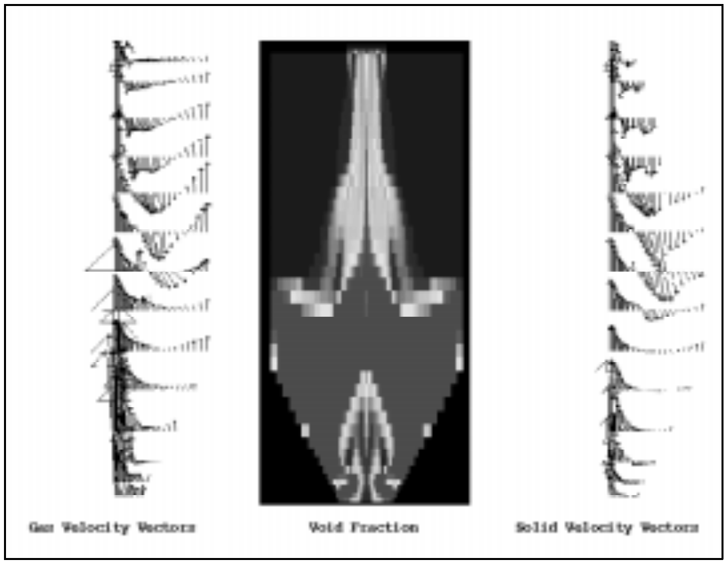

Figure 16: Westinghouse Run TP-M005-3 #12 at 6.5 seconds

MFIX is not able to simulate the spouting behavior of the He, et al. experiments (1995) because most of the bed is slumped. MFIX can and has predicted spouting bed behavior for other geometries and operating conditions (see, for example, the next section concerning Foster Wheeler Carbonizer Experiments). The only source of fluidizing air for the He, et al. (1995) experiments is the nozzle on the centerline. Outside of its influence, the bed material is packed and immobile like soil. The densely packed bed forms a cylinder through which the spout emerges. Next to the spout is a region where the bed material is in incipient flow. One large, much-investigated

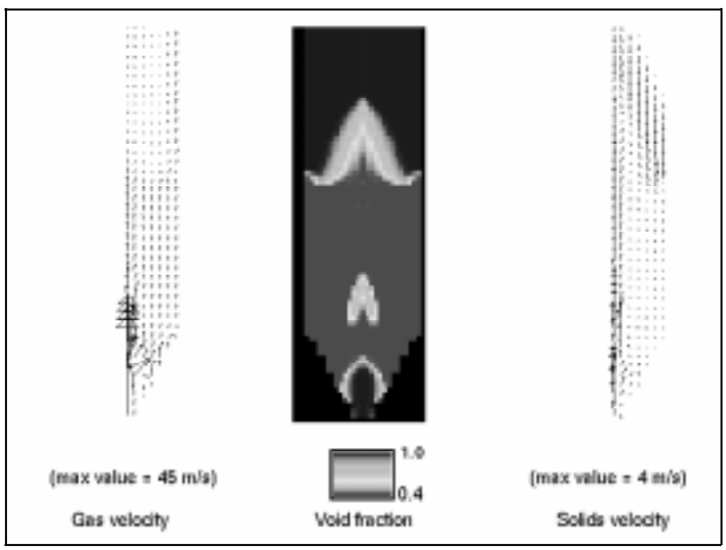

Figure 17: Spouting Bed Simulation: Jet Velocity = 44.9 m/s

question in the soil mechanics literature is the formulation of a stress tensor expression for such a dense, incipient, granular flow. Such a physical description is absent in MFIX. Instead, the slumped bed material is treated by MFIX as a very viscous liquid. The resulting simulations predict a solids circulation cell and solids pressure that cause the bed material to impinge on the nascent spout, pinch it off, and form a jetting/bubbling bed. For those experiments in which MFIX correctly predicts spouting behavior, no slumped bed exists because the vessel itself is too narrow to allow it. Thus, all of the bed material is fluidized, and none is in incipient flow. This situation is described well by the physical assumptions in MFIX.

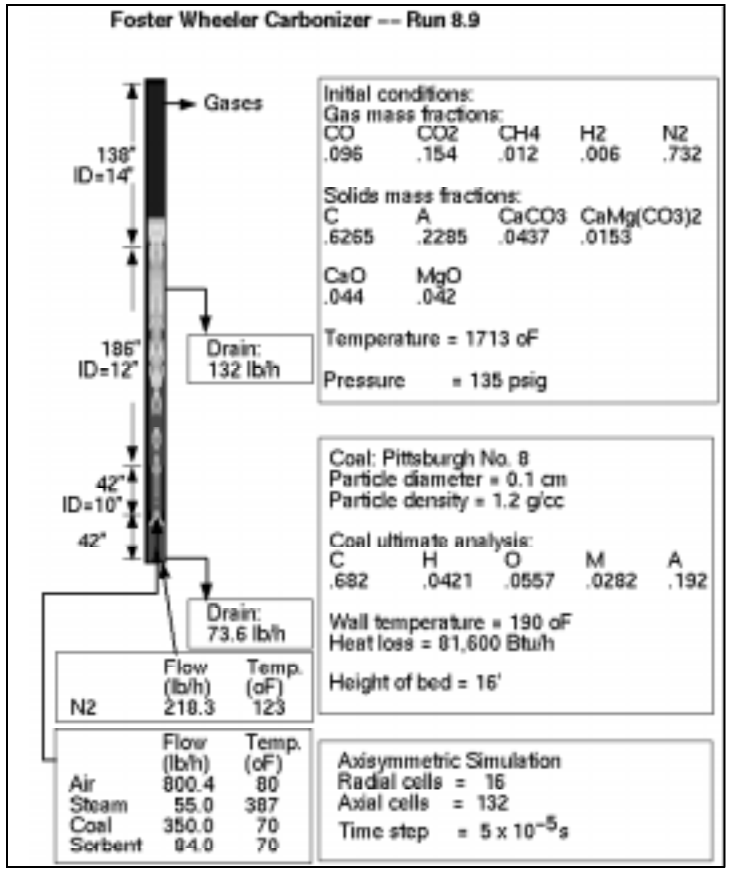

Figure 18: Fan (1995a)

Foster Wheeler Development Corporation (FWDC) 10" Carbonizer Experimental Run #TR8.9 (1995):

MFIX simulated FWDC Run #TR8.9 - a hot, pressurized, coal gasifier. Figure 18, FWDC Carbonizer Run #TR8.9 (1995), shows the geometry and operating conditions. Originally the simulation used a 0.025 cm average particle size, which was based on the injected solids size distribution. With that average particle size, the simulation predicted a spouting fluidization regime, which contradicted the experience and intuition of the Foster Wheeler personnel. The simulation was run a second time with the particle size increased to 0.1 cm based on the bottom ash size distribution, which was considered to be more representative of the actual particle sizes in the gasifier than was the size distribution of the injected solids. The resulting fluidization behavior was jetting/bubbling, which affirmed the intuition of Foster Wheeler personnel. The preliminary predicted and experimental exit-gas compositions are compared in the following Table on a dry mole % basis:

Gas Species	Experiment	Model
CO	9.03	5.72
CO_2	9.24	9.26
CH_4	1.92	5.47
H_2	7.89	5.90
N_2	68.70	73.65

These model-results for the gas composition for this second simulation, in which the flow regime is jetting/bubbling, are similar to those for the first simulation, in which the flow regime is spouting. Accordingly, the extra CH_4 and insufficient CO and H_2 as predicted by MFIX are probably caused by the rate for the reduction of CO by H_2O being too large rather than being caused by incorrect hydrodynamics.

Summary

The current MFIX validation study with Foster Wheeler uses four experimental investigations featuring a variety of geometries and operating conditions: Yang and Keairns (1980); Schmidt, et al. (1988); He, et al. (1995); and Foster Wheeler Development Corporation 10" Carbonizer Experimental Run #TR8.9, (Fan, October 1995a). The validation runs show that MFIX predicts well the bubble size, but the bubble often has an unphysical spike on its leading edge. The predicted jet penetration height and jet angle from two-dimensional simulations are close to the experimental values, but the predicted frequency with which a bubble forms above a jet is twice the experimental result. The MFIX predictions for spouting beds are problematic because MFIX does not consider dense, incipient flows. MFIX simulates well the hydrodynamic behavior of the Foster Wheeler 10" carbonizer whenever the average particle size is based on the bottom ash size distribution. The exit gas composition for the carbonizer depends more on the correct reaction rates than on the correct fluidization regime. The reaction rate parameters in MFIX can be adjusted to yield a better fit to the Foster Wheeler carbonizer data. Throughout, the desirability of increasing the computational speed of MFIX is clear.

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